Microstructural effects on strain localization in a multiscale model for hydro-mechanical coupling

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Abstract The formulation and implementation of a double-scale finite element model for hydromechanical coupling in the framework of the finite element squared method has allowed studying macroscale boundary value problems in a poromechanical continuum. The macroscale constitutive relations are directly derived from the micromechanical interaction between fluid and solid microstructure, captured in representative elementary volumes. The application of this model in the simulation of a biaxial test and a gallery excavation problem is presented here to give examples of the model in strain localization problems. While using simple micromechanical models, the results demonstrate the ability of the model to provide complex macroscale material behaviour, that controls the initiation and development of the strain localization.

1 Introduction

The modelling of micromechanical behaviour of geomaterials has provided means to describe material behaviour based on its microstructural constituents. This has

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allowed phenomenological constitutive laws for continuous media to be replaced by a direct simulation of the interaction between its microstructural constituents and different phases. However, the application of these microscale models in direct numerical simulations of macroscale problems can lead to excessive computational loads, as the length scale of common macroscale problems can be several orders of magnitude larger than the length scale of the microstructural constituents. To overcome this issue, the different scales can be treated in separate computations that are coupled in a homogenization scheme, using the homogenized material behaviour of so-called representative elementary volumes (REV) as the local material behaviour of a continuum description of the macroscale problem. As such, coupling between the scales of observation is used to take account of the microstructure in an averaged sense.

This paper presents some of the recent advances in the doublescale modelling of hydromechanical coupling in the framework of computational homogenization. A finite element squared (FE^2) formulation is used to derive the poromechanical continuum behaviour from a microscale model for microstructural solid-fluid interaction. After a general introduction of the modelling concept, examples of numerical simulations of laboratory tests and engineering structures are given. The examples are used to demonstrate the results obtained with the model and highlight the interplay between microstructural characteristics and macroscale initiation and propagation of strain localization.

2 The doublescale model

On the macroscale, a poromechanical continuum is formulated, of which the mechanical part of the solution of the macroscale boundary value problem is regularized by a local second gradient paradigm [8, 3]. This implicitly prescribes the internal length scale, needed for computations of softening behaviour without mesh dependency. For the second gradient part of the material behaviour, a linear-elastic constitutive relation is used [11, 2, 3], whereas the classical HM-coupled part is derived by means of computational homogenization from the computed equilibrium state of the REV [5]. For each integration point in the FE computation, an equilibrium state of the corresponding REV is computed with boundary conditions dictated by the local kinematics of the iterative macroscale test solution. From this equilibrium state, a consistent tangent operators (with respect to the rate of change of the test solution kinematics) and the homogenized response (stress state, fluid content, fluid mass flux) is derived by means of computational homogenization [5]. In this way, the REV boundary conditions and the computational homogenization for the coupling from macro to micro and from micro to macro respectively.

A microscale model was formulated in continuation of the model developments in Grenoble [1, 7, 10], in which the microstructure is modeled as an assembly of solid grains using the finite element method. Grains are considered elastic and the interfaces between grains are modelled by triple-noded interface elements to account for relative displacements between grains and fluid flow in the resulting interface channels (Figure 1). Cohesive normal and tangential traction components T_n

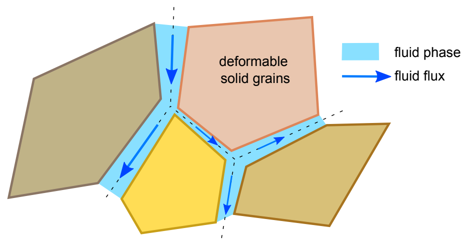

Fig. 1 Microscale model concept of elastic grains separated by cohesive interfaces [4].

and T_t, acting over the interfaces between the grains, are described independently as functions of components Δu_n and Δu_t of the relative displacement between sides of the interface. A simple damage formulation is used for interface cohesion, introducing softening in the computed material behaviour (Figure 2). Although coupling between the two components of cohesion are not used in the microscale formulation, confining stress-dependency of the macroscale behaviour is found as an effect of interlocking of the grains at the microscale. Nevertheless, interface mechanical behaviour can easily be modified within the same framework of homogenization.

A pore channel network is formed by the interfaces between the grains, allowing pore fluid to percolate. Fluid flow is modelled by means of one-dimensional channel elements with equivalent hydraulic conductivity, based on Poiseuille flow between smooth parallel plates. In addition, the water content depends on the relative volume of the pore space that is formed by the opened interfaces.

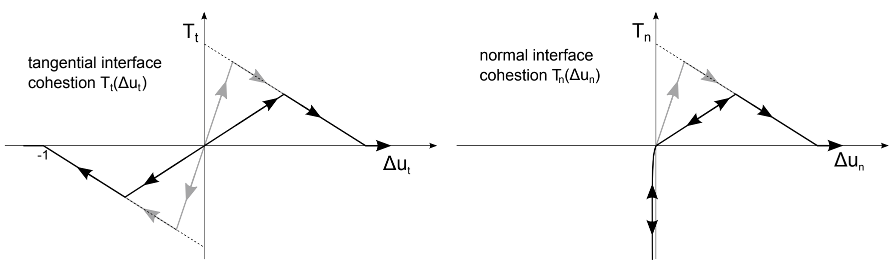

Fig. 2 Interface damage model for normal and tangential cohesion between grains over the interface . Penalization is used to account for contact between grains under local compression [5].

Upscaling from the equilibrated microscale model to the local macroscale response terms and constitutive behaviour is obtained through computational homogenization [9, 12]. This framework was extended to the case of hydromechanical coupling in the steady-state microscale model presented above, and provides the homogenized response of the REV as well as the tangent operators consistent to the current loading direction [5]. The classical, first order part of the material behaviour is thereby derived completely from the micromechanical model, without the need for determining derivatives of state by means of numerical perturbations.

3 Simulations of a biaxial compression test

A biaxial compression test of a fluid-saturated material was modeled under transient conditions. The REV characterizing the material microstructure was varied in orientation with respect to the sample orientation to have different orientations of anisotropy. No confining pressure was applied and samples were drained at the bottom and top; a weak element was introduces at both lower corners to attract the initiation of strain localization. The specific microstructure, including an average elongation to represent the effect of a bedding plane, is rotated between the different samples to obtain different orientations of the anisotropic behaviour with respect to the loading direction.

Figure 3 shows the deviatoric strain fields of four of these tests in post-peak conditions. A deformed microstructure is given for each test, corresponding to a characteristic point A in the shear band that has developed. Mesh-independent results for shear bands are obtained through the regularization of the macroscale solution.

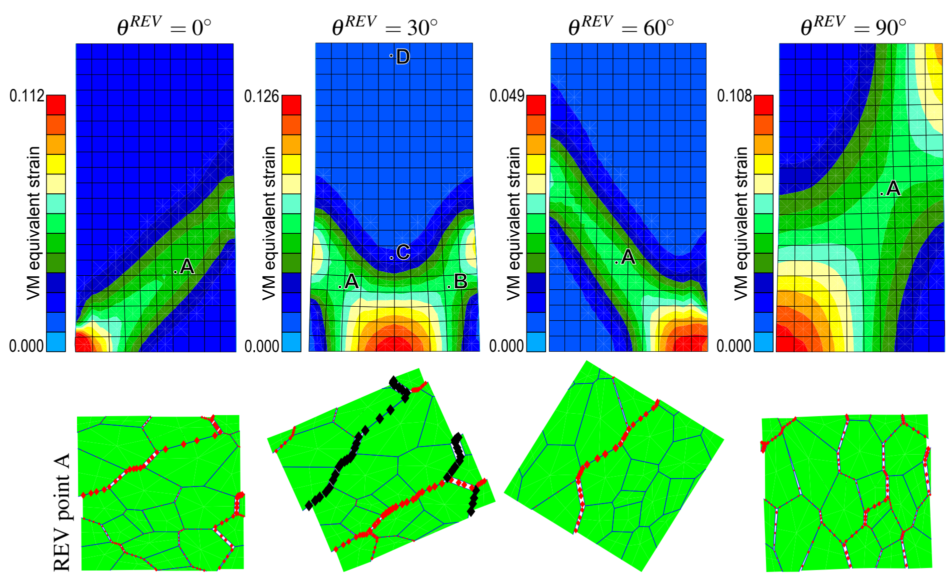

Fig. 3 Deformed macroscale samples and corresponding microstructures after loading at axial strain rate $\dot{\varepsilon}_a = 1 \times 10^{-8}$. Symbols ♦ and ♦ represent the interface state in softening and decohesion respectively [5].

4 Simulations of the excavation of a tunnel

The excavation damaged zone around a deep tunnel was modeled. The excavation process in a 2D plane strain model is simulated by gradually reducing the initial stress state ($\sigma_v = -12.7$ MPa, $\sigma_h = -16.1$ MPa, $p = 4.7$ MPa) at the future tunnel wall, until zero-stress state is reached at the tunnel wall after 28 days. Four different microstructures are used to characterize the material microstructure, generated using a Voronoï-based algorithm [6]. Although not large enough to give statistically representative elementary volumes, the specific realizations of microstructures represent macroscale material behaviour related to their specific type of granular assembly and grain geometry and the resulting difference in macroscale behaviour is studied in relation with initiation of strain localization.

Figure 4 shows four REVs with microstructure, rotated to align the peak strength with the reference axes. The macroscale strain rate fields at the end of the excavation are given for simulations with each of these microstructures. The strain rate fields show the localized activity at the final stage of excavation, controlled directly by the microstructure in the REV. Building further on these observations, the influence of the microstructure on the macroscale initiation of strain localization can be explored.

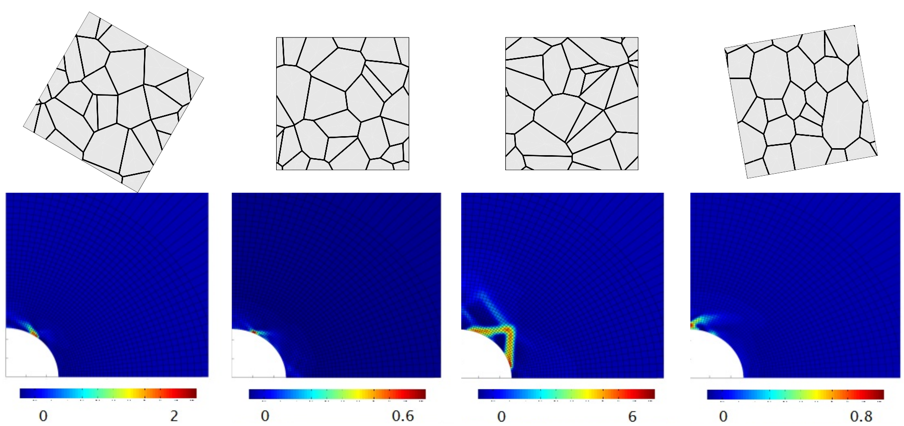

Fig. 4 Initiation of strain localization for material behaviour derived from different microstructures. Colorscale represents deviatoric strain rate, normalized against relative stage of unloading on tunnel wall [6].

In addition to the examples of strain localization given above, the presented simulations can be used to study the hydromechanical coupling in the doublescale model. As part of the hydromechanical coupled behaviour, the macroscale fluid transport phenomena can be derived from the micromechanical model of solid-fluid interaction. Both controlled by the deformation of the microstructure, the evolution of the permeability tensor and the zones of strain localization can be related.

5 Conclusions

The development and implementation of a finite element squared method for hydromechanical coupling has provided a doublescale approach for modelling strain localization in fluid-saturated rock-like materials. The given examples demonstrate the ability of the model to account for complex macroscale material behaviour, including anisotropy and softening. The regularization of the solution by a local second gradient paradigm provides mesh-objective macroscale solution to problems involving strain localization. As such, a conceptual demonstration of the application of a finite element squared method for hydromechanical coupling is given for problems at semi-engineering scale.

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